10088425

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NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2	Apr 08	"Ask CAS" for self-help around the clock
NEWS 3	Jun 03	New e-mail delivery for search results now available
NEWS 4	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 5	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 6	Aug 26	Sequence searching in REGISTRY enhanced
NEWS 7	Sep 03	JAPIO has been reloaded and enhanced
NEWS 8	Sep 16	Experimental properties added to the REGISTRY file
NEWS 9	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 10	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS 11	Oct 24	BEILSTEIN adds new search fields
NEWS 12	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 13	Nov 18	DKILIT has been renamed APOLLIT
NEWS 14	Nov 25	More calculated properties added to REGISTRY
NEWS 15	Dec 04	CSA files on STN
NEWS 16	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 17	Dec 17	TOXCENTER enhanced with additional content
NEWS 18	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 19	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 20	Feb 13	CANCERLIT is no longer being updated
NEWS 21	Feb 24	METADEX enhancements
NEWS 22	Feb 24	PCTGEN now available on STN
NEWS 23	Feb 24	TEMA now available on STN
NEWS 24	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS 25	Feb 26	PCTFULL now contains images
NEWS 26	Mar 04	SDI PACKAGE for monthly delivery of multifile SDI results
NEWS 27	Mar 19	APOLLIT offering free connect time in April 2003
NEWS 28	Mar 20	EVENTLINE will be removed from STN
NEWS 29	Mar 24	PATDPAFULL now available on STN
NEWS 30	Mar 24	Additional information for trade-named substances without structures available in REGISTRY
NEWS 31	Apr 11	Display formats in DGENE enhanced
NEWS 32	Apr 14	MEDLINE Reload
NEWS 33	Apr 17	Polymer searching in REGISTRY enhanced
NEWS 34	Apr 21	Indexing from 1947 to 1956 being added to records in CA/CAPLUS
NEWS 35	Apr 21	New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX
NEWS 36	Apr 28	RDISCLOSURE now available on STN
NEWS 37	May 05	Pharmacokinetic information and systematic chemical names added to PHAR

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 NEWS EXPRESS  April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT
               MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
               AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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FILE 'HOME' ENTERED AT 12:21:31 ON 10 MAY 2003

=> fil reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'REGISTRY' ENTERED AT 12:21:53 ON 10 MAY 2003
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STRUCTURE FILE UPDATES:     9 MAY 2003  HIGHEST RN 513416-44-9
DICTIONARY FILE UPDATES:    9 MAY 2003  HIGHEST RN 513416-44-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
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L1      STRUCTURE UPLOADED

=> fil casreact
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10088425

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.40	0.61

FILE 'CASREACT' ENTERED AT 12:22:12 ON 10 MAY 2003
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FILE CONTENT:1907 - 4 May 2003 VOL 138 ISS 18

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

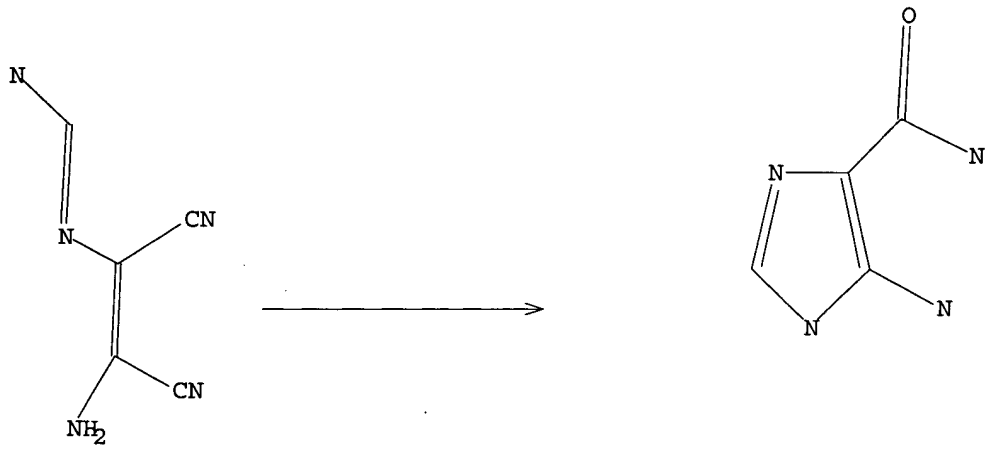
Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=>
Uploading 10088425.str

L2 STRUCTURE UPLOADED

=> d l2
L2 HAS NO ANSWERS
L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 12:22:41 FILE 'CASREACT'

10088425

SCREENING COMPLETE - 3 REACTIONS TO VERIFY FROM 2 DOCUMENTS

100.0% DONE 3 VERIFIED 3 HIT RXNS 2 DOCS
SEARCH TIME: 00.00.01

L3 2 SEA SSS FUL L1 (3 REACTIONS)

=> d l3 ibib abs hitstr
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number. SCAN must be entered on the same line as DISPLAY, e.g., D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with CA reference information (SO, PY). (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction Summary for all hit reactions and fields containing hit terms
OCC -------- All hit fields and the number of occurrences of the hit terms in each field. Includes total number of HIT, PATH, SPATH reactions. Labels reactions that have incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long path". Displays all hit reactions, except those

whose steps are totally included within another hit reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

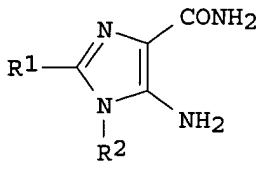
ENTER DISPLAY FORMAT (FCRDREF):all

L3 ANSWER 1 OF 2 CASREACT COPYRIGHT 2003 ACS
AN 134:252338 CASREACT
TI Processes for the preparation of 4(5)-amino-5(4)-carboxamidoimidazoles and intermediates thereof
IN Shibasaki, Hiroaki; Nagasaki, Fumihiko; Takase, Mitsuru; Yamazaki, Satoru; Ishii, Yutaka; Oohata, Kimihiko
PA Nippon Soda Co., Ltd., Japan; Ibaraki Kasei Co., Ltd.
SO PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
IC ICM C07D233-90
ICS C07C257-14
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001021592	A1	20010329	WO 2000-JP6397	20000920
	W: CN, IN, KR, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	JP 2001151760	A2	20010605	JP 1999-330103	19991119
	JP 2001302609	A2	20011031	JP 2000-116218	20000418
	JP 2001158776	A2	20010612	JP 2000-284780	20000920
	EP 1215206	A1	20020619	EP 2000-961096	20000920
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				

PRAI JP 1999-264818 19990920
JP 1999-330103 19991119
JP 2000-116218 20000418
WO 2000-JP6397 20000920
OS MARPAT 134:252338

GI



I

AB The invention provides novel processes for prepg. efficiently compds. of general formula (I) (wherein R1 and R2 are each independently hydrogen, optionally substituted C1-10 alkyl, C3-14 hydrocarbyl bearing an alicyclic skeleton, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, optionally substituted heterocyclyl, optionally substituted heterocyclylalkyl, N-optionally substituted carbamoyl, or alkoxycarbonyl) and intermediates thereof. Compds. of general formula I can be prepd. by subjecting compds. of general formula R2NHC(R1):NC(CN):C(NH2)CN (II; R1 and R2 are defined above) and/or salts thereof to cyclization hydrolysis in an aq. basic soln. Further, compds. of general formula II can be prepd. from industrially easily available diaminomaleonitrile in a high yield. The compds. I are useful as intermediates for agrochems. and drugs, e.g. dacarbazine and temozoromide (anticancer agent) and urazamide (liver-protective agent). Thus, 50 mL H2O and 43.0 g 25% NaOH were added to 8.0 g N-(2-amino-1,2-dicyanovinyl)formamidine and refluxed for 2 h, cooled to room temp., neutralized with 35% HCl to pH 7, concd. to dryness, treated with ethanol, and filtered for removing the insol. salt. The filtrate was treated with activated charcoal, filtered, and concd. to give a soln. of 4(5)-aminoimidazole-5-carboxamide (III) which was adjusted to pH .ltoreq.3 and cooled at .ltoreq.10.degree.. The pptd. crystals were collected by filtration and dried to give 84% III.HCl.

ST aminoimidazolecarboxamide prepn intermediate anticancer; aminodicyanovinylformamidine cyclization aminoimidazolecarboxamide

IT Liver, disease
(hepatoprotective agents; prepn. of aminocarboxamidoimidazoles as intermediates for anticancer and liver-protective agents by cyclization of (aminodicyanovinyl)formamidine derivs.)

IT Antitumor agents
Cyclization
(prepn. of aminocarboxamidoimidazoles as intermediates for anticancer and liver-protective agents by cyclization of (aminodicyanovinyl)formamidine derivs.)

IT 75-12-7, Formamide, reactions 78-82-0, Isobutyronitrile 109-74-0, Butyronitrile 122-51-0, Triethyl orthoformate 149-73-5, Trimethyl orthoformate 1187-42-4, Diaminomaleonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of aminocarboxamidoimidazoles as intermediates for anticancer and liver-protective agents by cyclization of (aminodicyanovinyl)formamidine derivs.)

IT 123060-28-6P, Methyl N-(2-amino-1,2-dicyanovinyl)formimidate 133123-63-4P, Ethyl N-(2-amino-1,2-dicyanovinyl)formimidate 331282-40-7P, N-(2-Amino-1,2-dicyanovinyl)formamidine 331282-41-8P, N-(2-Amino-1,2-dicyanovinyl)isobutyramidine hydrochloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of aminocarboxamidoimidazoles as intermediates for anticancer

and liver-protective agents by cyclization of (aminodicyanovinyl)formamidine derivs.)

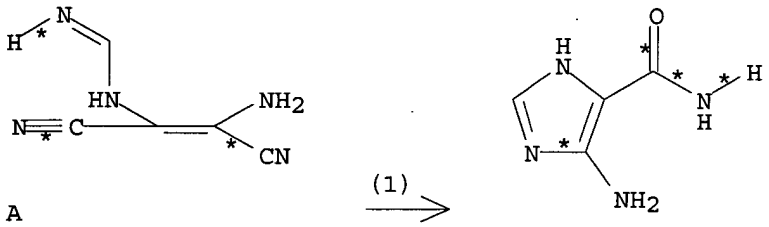
IT 72-40-2P, 4-Aminoimidazole-5-carboxamide hydrochloride 90521-73-6P, 5-Amino-2-propyl-1H-imidazole-4-carboxamide 227078-19-5P, 5-Amino-2-isopropyl-1H-imidazole-4-carboxamide 331282-42-9P, N-(2-Amino-1,2-dicyanovinyl)butyramidine hydrochloride
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of aminocarboxamidoimidazoles as intermediates for anticancer and liver-protective agents by cyclization of (aminodicyanovinyl)formamidine derivs.)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Booth, B; Jounal of Heterocyclic Chemistry 1994, V31(2), P345
(2) Booth, B; Tetrahedron Letters 1993, V34(34), P5503 CAPLUS
(3) Kyowa Gas Chemical Ind Co Ltd; JP 5119127 A 1976
(4) Weigert, F; US 3778446 A 1973 CAPLUS

RX(1) OF 4 **A** ===> **B**



A

(1)

● HCl

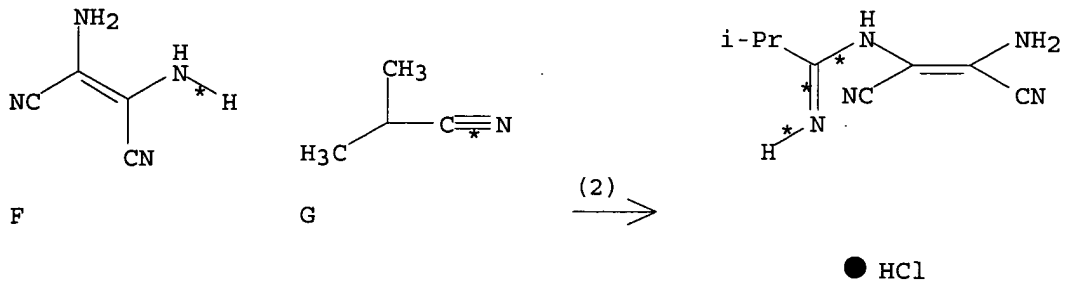
B
YIELD 84%

RX(1) RCT A **331282-40-7**

STAGE(1)
RGT C 1310-73-2 NaOH
SOL 7732-18-5 Water

STAGE(2)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water
PRO B **72-40-2**

RX(2) OF 4 F + G ===> H...

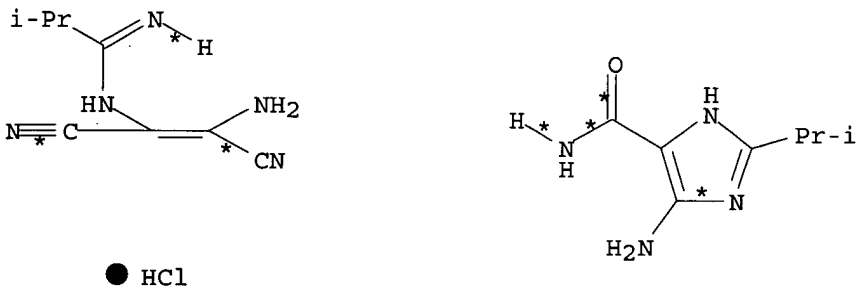


F G (2) ● HCl

H

RX(2) RCT F 1187-42-4, G 78-82-0
RGT D 7647-01-0 HCl
PRO H 331282-41-8

RX(3) OF 4 ...**H** ===> **I**



● HCl

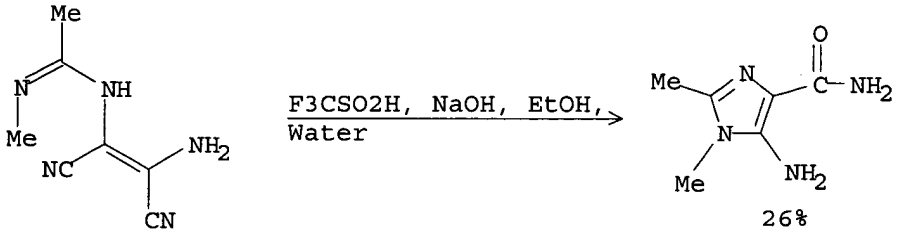
H (3) I
YIELD 70%

RX(3) RCT H **331282-41-8**
RGT C 1310-73-2 NaOH
PRO I **227078-19-5**
SOL 7732-18-5 Water

=> d l3 2

L3 ANSWER 2 OF 2 CASREACT COPYRIGHT 2003 ACS

RX(5) OF 78

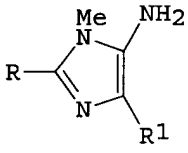


26%

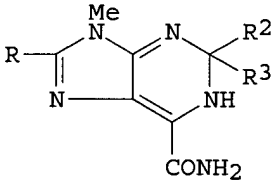
REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (7), 1521-6; 1987

=> d l3 2 all

L3 ANSWER 2 OF 2 CASREACT COPYRIGHT 2003 ACS
AN 108:150133 CASREACT
TI Chemistry of nitrilium salts. Part 4. Some reactions of 5-amino-4-(C-cyanoformimidoyl)imidazoles obtained from nitrilium trifluoromethanesulfonate salts and diaminomaleonitrile
AU Booth, Brian L.; Coster, Ronald D.; Fernanda, M.; Proenca, J. R. P.
CS Inst. Sci. Technol., Univ. Manchester, Manchester, M60 1QD, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (7), 1521-6
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
CC 26-9 (Biomolecules and Their Synthetic Analogs)
GI



II

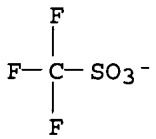


III

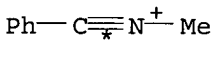
AB Diaminomaleonitrile reacted readily with RC.tplbond.N+Me O3-SCF3 (R = Me, Ph) to give MeNHC+RNHC(CN):C(CN)NH2 O3-SCF3 (I; R = Me, Ph), which on base treatment under different conditions gave imidazoles II [R1 = cyano, CONH2, C(CN):NH]. I reacted with aldehydes and ketones at room temp. to give trifluorometanesulfonate salts of dihydropurines III [R = Me, Ph; R2 = Me, H; R3 = Me, Ph; R2R3 = (CH2)4]. Similarly II [R = Me, R1 = C(CN):NH] reacted with aldehydes, ketones, 1,2- and 1,3-diketones and keto esters to give dihydropurines III (R = R2 = Me, R3 = Me, Et, Ph, COMe, CH2CO2Et, CO2Et, CH2COMe; R = Me, R2 = Ph, R3 = H, Bz) some of which oxidized in air to purines.
ST diaminomaleonitrile nitrilium addn; cyanoformimidoylimidazoleamine prepn aldehyde ketone cycloaddn; imidazoleamine carbamoyl cyano; purine dihydro
IT Cycloaddition reaction
(of (cyanoformimidoyl)imidazoleamines with aldehydes and ketones,

purines from)
IT Addition reaction
(of diaminomaleonitrile with nitrilium salts)
IT 76893-86-2 76893-90-8, N-Methylbenzonitrilium triflate
RL: RCT (Reactant); RACT (Reactant or reagent)
(addn. reaction of, with diaminomaleonitrile, amidinium salts from)
IT 1187-42-4, Diaminomaleonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(addn. reactions of, with nitrilium salts)
IT 367-57-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn. reaction of, with (cyanoformimidoyl)imidazoleamine deriv., purine deriv. from)
IT 78-93-3, reactions 123-54-6, reactions 123-72-8 134-81-6 141-97-9 431-03-8, Butane-2,3-dione 617-35-6, Ethyl pyruvate
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn. reaction of, with (cyanoformimidoyl)imidazoleamine derivs., purine deriv. from)
IT 67-64-1, reactions 98-86-2, reactions 100-52-7, reactions 108-94-1, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn. reactions of, with (cyanoformimidoyl)imidazoleamines and amidinium salts, purines from)
IT 112995-37-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and cyclization of, with acetone, purine from)
IT 112995-31-0P 112995-33-2P 112995-35-4P 113684-62-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and cyclization of, with aldehydes and ketones, purines from)
IT 80052-80-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cycloaddn. reactions of, with aldehydes, ketones and keto esters, purines from)
IT 80052-89-7P 80052-90-0P 80052-92-2P 80052-93-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidn. of)
IT 78750-93-3P 80052-79-5P 80052-81-9P 80052-82-0P 80052-83-1P 80052-85-3P 80052-86-4P 80052-87-5P 80052-88-6P 80052-91-1P 112995-38-7P 112995-40-1P 112995-41-2P 112995-42-3P 112995-44-5P 112995-45-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RX(1) OF 78 2 A + 2 B ===> C + D...



2 A: CM 1



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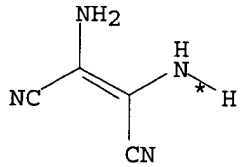
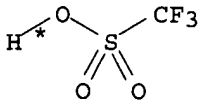
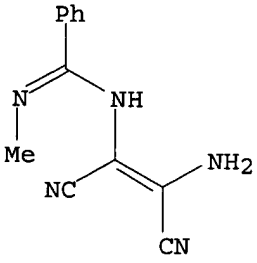


2 B

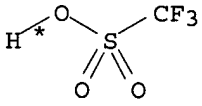
(1) ⟶



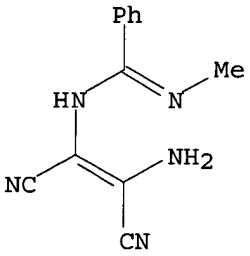
C: CM 1



C: CM 2



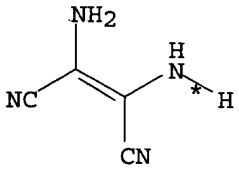
D: CM 1



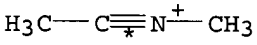
D: CM 2

RX(1) RCT A 76893-90-8, B 1187-42-4
PRO C 112995-31-0, D 112995-33-2
SOL 75-52-5 MeNO2
NTE 80% overall

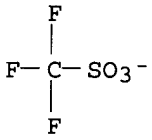
RX(2) OF 78 2 B + 2 F ===> G + H...



2 B

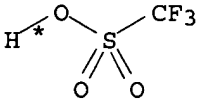


2 F: CM 1

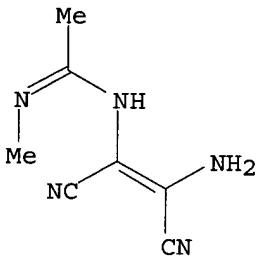


2 F: CM 2

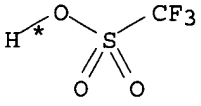
(2) ⟶



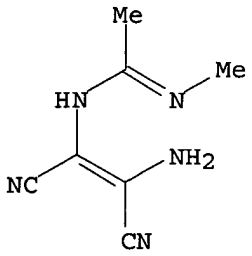
G: CM 1



G: CM 2



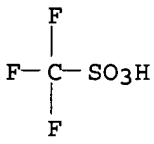
H: CM 1



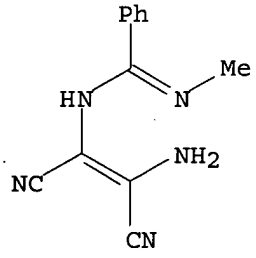
H: CM 2

RX(2) RCT B 1187-42-4, F 76893-86-2
PRO G 112995-35-4, H 113684-62-1
SOL 75-52-5 MeNO2
NTE 60% overall

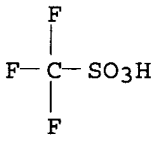
RX(3) OF 78 ...D + C ===> 2 I...



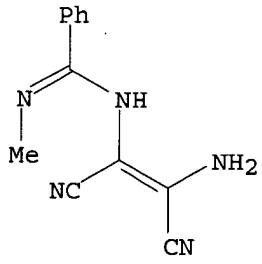
D: CM 1



D: CM 2

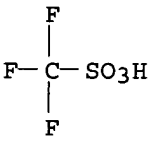


C: CM 1

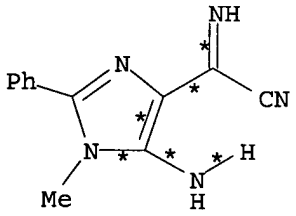


C: CM 2

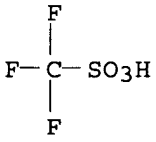
(3) →



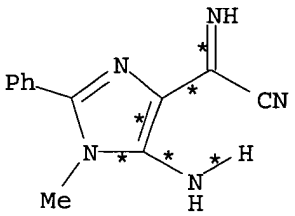
I: CM 1
YIELD 97%



I: CM 2
YIELD 97%



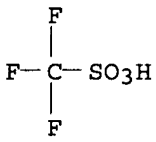
I: CM 1
YIELD 97%



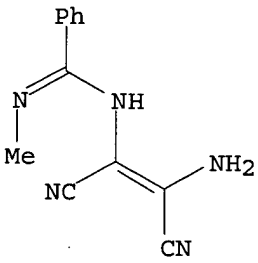
I: CM 2
YIELD 97%

RX(3) RCT D 112995-33-2, C 112995-31-0
PRO I 112995-37-6
SOL 75-52-5 MeNO2, 67-66-3 CHCl3

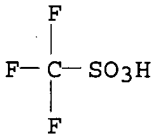
RX(4) OF 78 ...C + D ===> 2 K



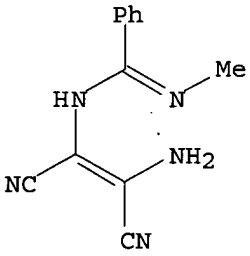
C: CM 1



C: CM 2

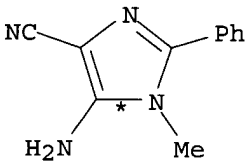


D: CM 1

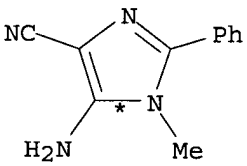


D: CM 2

(4) →



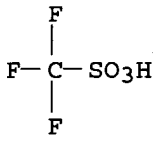
K
YIELD 50%



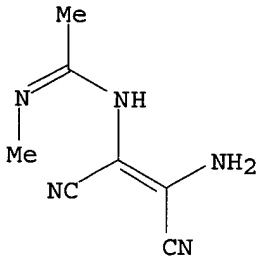
K
YIELD 50%

RX(4) RCT C 112995-31-0, D 112995-33-2
RGT L 1310-58-3 KOH
PRO K 112995-38-7
SOL 64-17-5 EtOH, 7732-18-5 Water

RX(5) OF 78 ...G ===> O

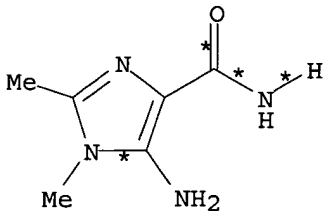


G: CM 1



G: CM 2

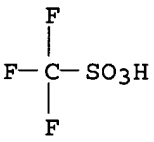
(5)



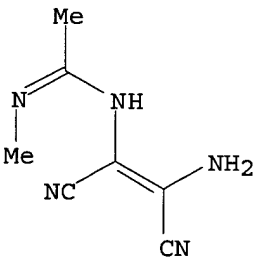
O
YIELD 26%

RX(5) RCT G **112995-35-4**
RGT P 1310-73-2 NaOH
PRO O **78750-93-3**
SOL 64-17-5 EtOH, 7732-18-5 Water

RX(6) OF 78 ...G ===> Q...

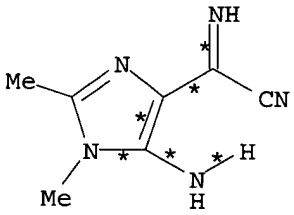


G: CM 1



G: CM 2

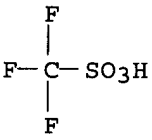
(6)



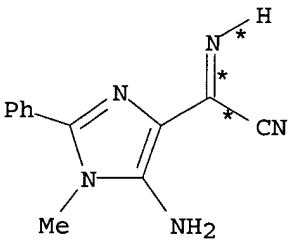
Q
YIELD 83%

RX(6) RCT G 112995-35-4
RGT R 497-19-8 Na2CO3
PRO Q 80052-80-8
SOL 7732-18-5 Water

RX(7) OF 78 ...I ===> K

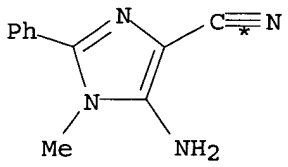


I: CM 1



I: CM 2

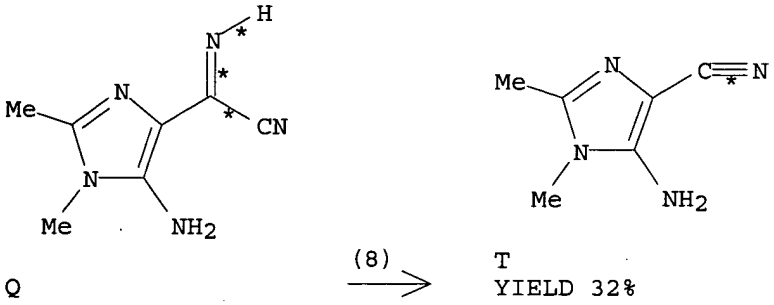
(7)



K

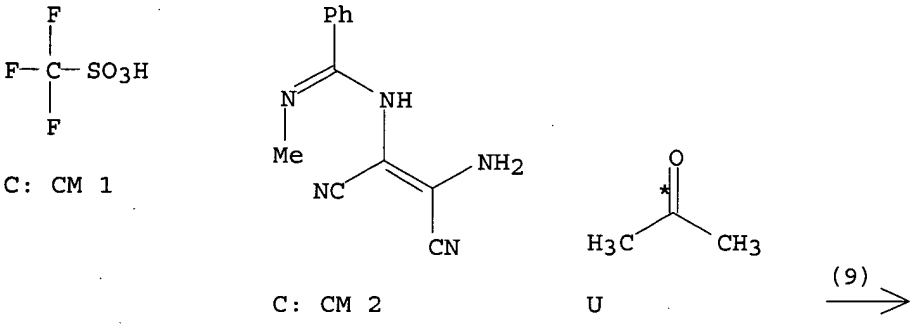
RX(7) RCT I 112995-37-6
RGT R 497-19-8 Na2CO3
PRO K 112995-38-7
SOL 7732-18-5 Water, 67-56-1 MeOH

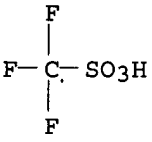
RX(8) OF 78 ...Q ===> T



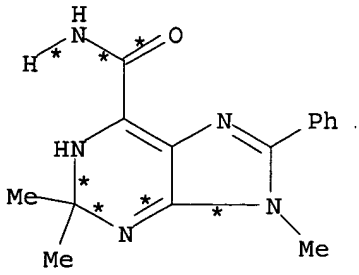
RX(8) RCT Q 80052-80-8
RGT P 1310-73-2 NaOH
PRO T 80052-79-5
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(9) OF 78 ...C + U ===> V





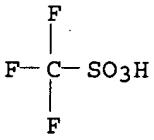
V: CM 1
YIELD 97%



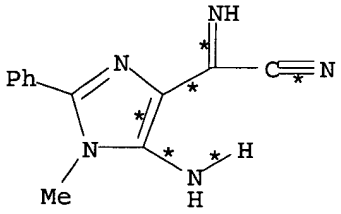
V: CM 2
YIELD 97%

RX(9) RCT C 112995-31-0, U 67-64-1
PRO V 112995-40-1

RX(10) OF 78 ...I ===> V

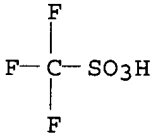


I: CM 1

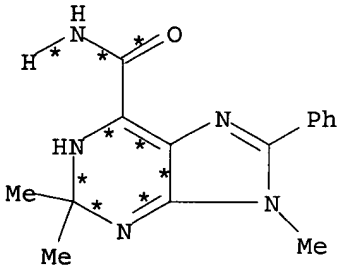


I: CM 2

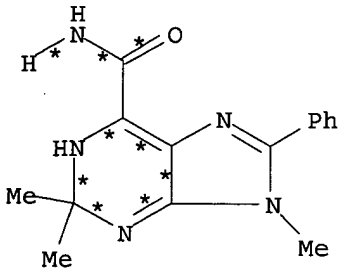
(10)



V: CM 1
YIELD 85%



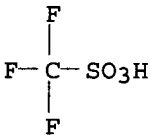
V: CM 2
YIELD 85%



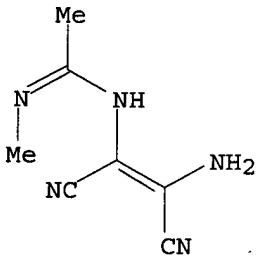
V: CM 2
YIELD 85%

RX(10) RCT I 112995-37-6
RGT U 67-64-1 Me2CO
PRO V 112995-40-1

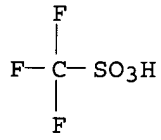
RX(11) OF 78 ...G + H + 2 W ===> 2 X



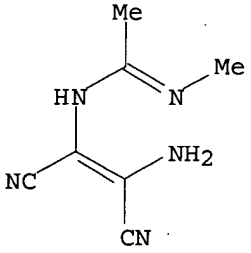
G: CM 1



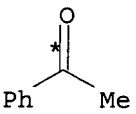
G: CM 2



H: CM 1

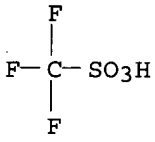


H: CM 2

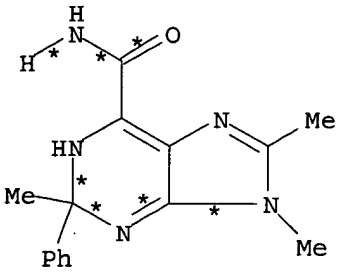


2 W

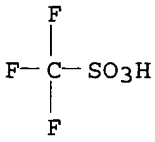
(11)



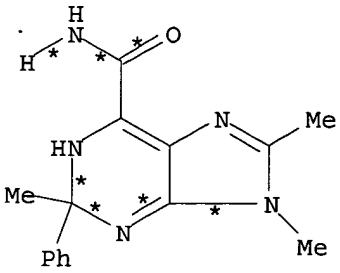
X: CM 1
YIELD 69%



X: CM 2
YIELD 69%



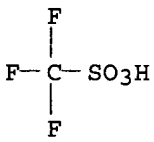
X: CM 1
YIELD 69%



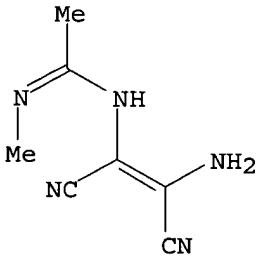
X: CM 2
YIELD 69%

RX(11) RCT G 112995-35-4, H 113684-62-1, W 98-86-2
RGT Y 110-86-1 Pyridine
PRO X 112995-42-3
SOL 98-86-2 Acetophenone

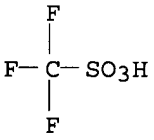
RX(12) OF 78 ...G + H + 2 Z ===> 2 AA



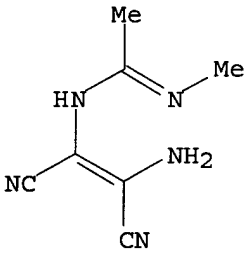
G: CM 1



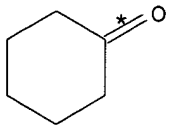
G: CM 2



H: CM 1

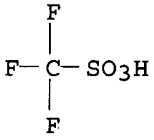


H: CM 2

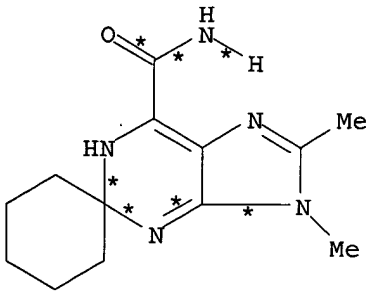


2 Z

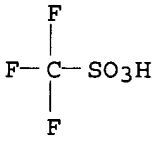
(12)



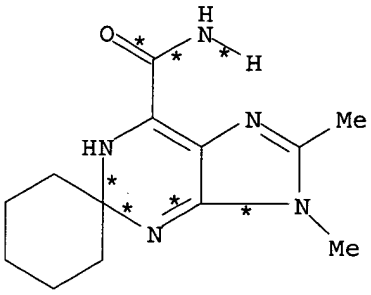
AA: CM 1
YIELD 50%



AA: CM 2
YIELD 50%



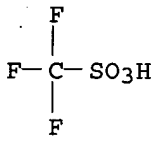
AA: CM 1
YIELD 50%



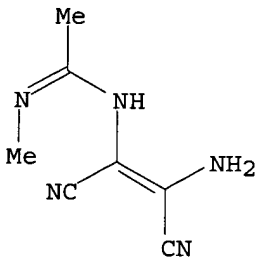
AA: CM 2
YIELD 50%

RX(12) RCT G 112995-35-4, H 113684-62-1, Z 108-94-1
RGT Y 110-86-1 Pyridine
PRO AA 112995-44-5
SOL 108-94-1 Cyclohexanone

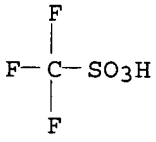
RX(13) OF 78 ...G + H + 2 AB ===> 2 AC



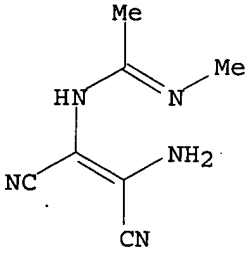
G: CM 1



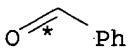
G: CM 2



H: CM 1

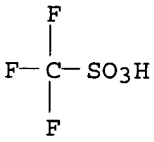


H: CM 2

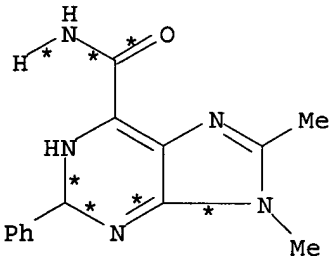


2 AB

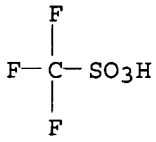
(13)



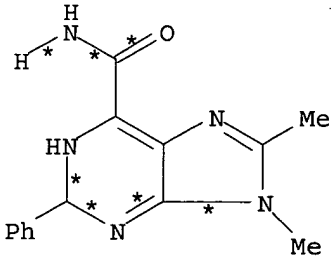
AC: CM 1
YIELD 60%



AC: CM 2
YIELD 60%



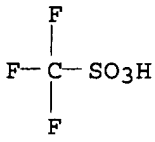
AC: CM 1
YIELD 60%



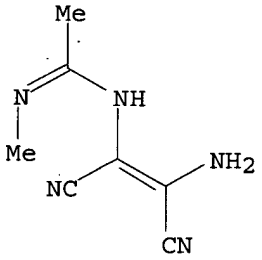
AC: CM 2
YIELD 60%

RX(13) RCT G 112995-35-4, H 113684-62-1, AB 100-52-7
RGT Y 110-86-1 Pyridine
PRO AC 112995-45-6
SOL 100-52-7 PhCHO

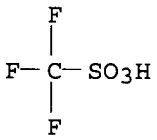
RX(14) OF 78 ...G + H + 2 U ===> 2 AD



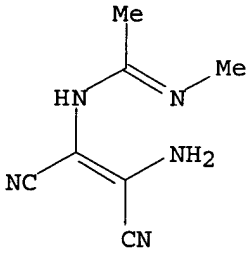
G: CM 1



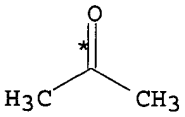
G: CM 2



H: CM 1

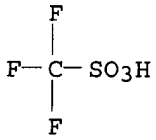


H: CM 2

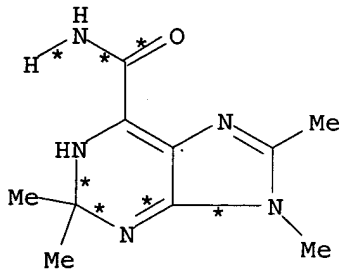


2 U

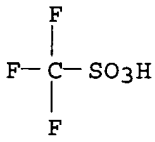
(14)



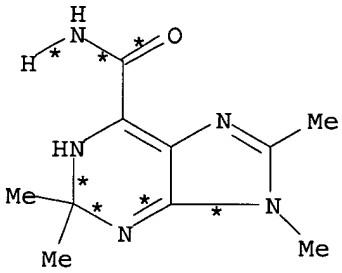
AD: CM 1
YIELD 80%



AD: CM 2
YIELD 80%



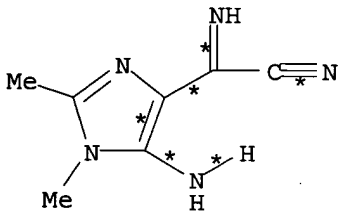
AD: CM 1
YIELD 80%



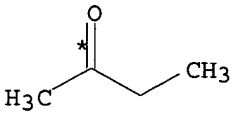
AD: CM 2
YIELD 80%

RX(14) RCT G 112995-35-4, H 113684-62-1, U 67-64-1
RGT Y 110-86-1 Pyridine
PRO AD 112995-41-2
SOL 67-64-1 Me2CO

RX(15) OF 78 ...Q + AE ===> AF

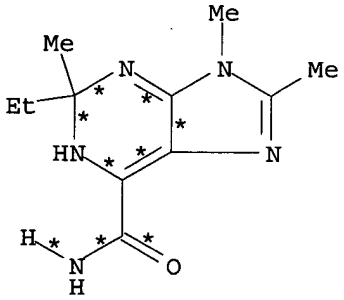


Q



AE

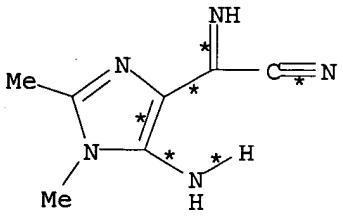
(15) ⟶



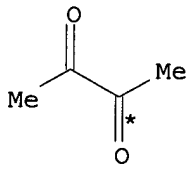
AF
YIELD 65%

RX(15) RCT Q 80052-80-8, AE 78-93-3
PRO AF 80052-87-5
SOL 78-93-3 EtCOMe

RX(16) OF 78 ...Q + AG ===> AH...

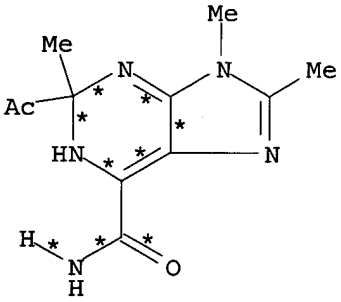


Q



AG

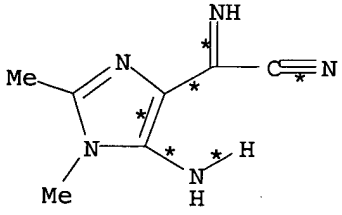
(16)



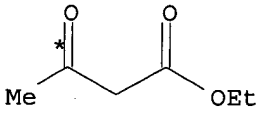
AH
YIELD 67%

RX(16) RCT Q 80052-80-8, AG 431-03-8
PRO AH 80052-89-7
SOL 64-17-5 EtOH

RX(17) OF 78 ...Q + AI ===> AJ...

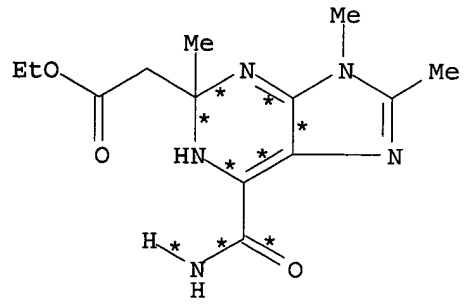


Q



AI

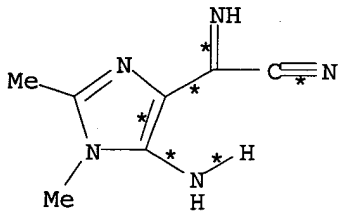
(17)



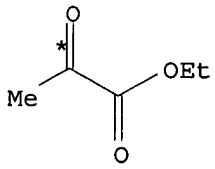
AJ
YIELD 80%

RX(17) RCT Q 80052-80-8, AI 141-97-9
PRO AJ 80052-90-0
SOL 64-17-5 EtOH

RX(18) OF 78 ...Q + AK ===> AL

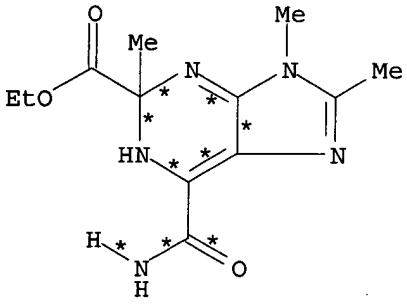


Q



AK

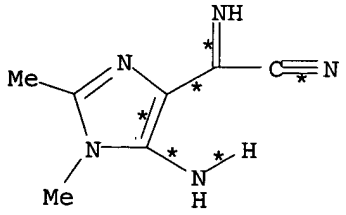
(18)



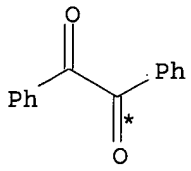
AL
YIELD 54%

RX(18) RCT Q 80052-80-8, AK 617-35-6
PRO AL 80052-91-1
SOL 64-17-5 EtOH

RX(19) OF 78 ...Q + AM ===> AN...

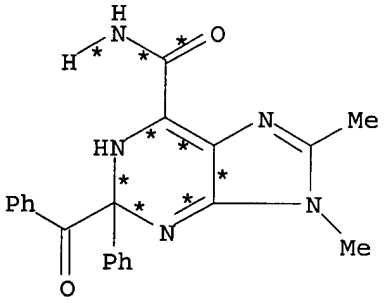


Q



AM

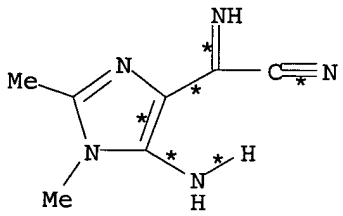
(19)



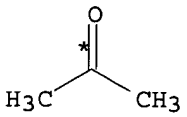
AN
YIELD 93%

RX(19) RCT Q 80052-80-8, AM 134-81-6
PRO AN 80052-92-2
SOL 64-17-5 EtOH

RX(20) OF 78 ...Q + U ===> AO

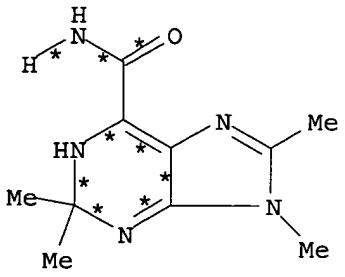


Q



U

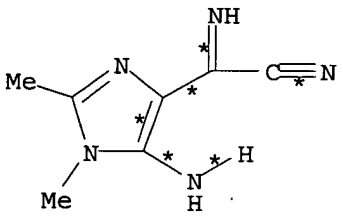
(20)



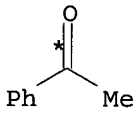
AO
YIELD 90%

RX(20) RCT Q 80052-80-8, U 67-64-1
PRO AO 80052-81-9
SOL 67-64-1 Me2CO

RX(21) OF 78 ...Q + W ===> AP

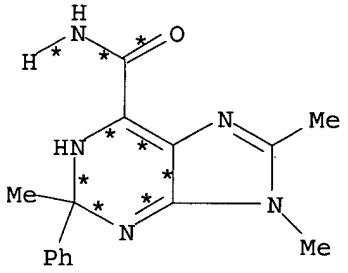


Q



W

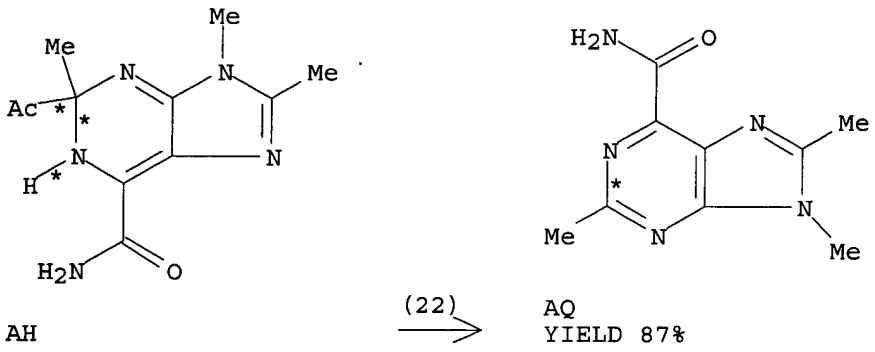
(21)



AP
YIELD 82%

RX(21) RCT Q 80052-80-8, W 98-86-2
PRO AP 80052-88-6
SOL 98-86-2 Acetophenone

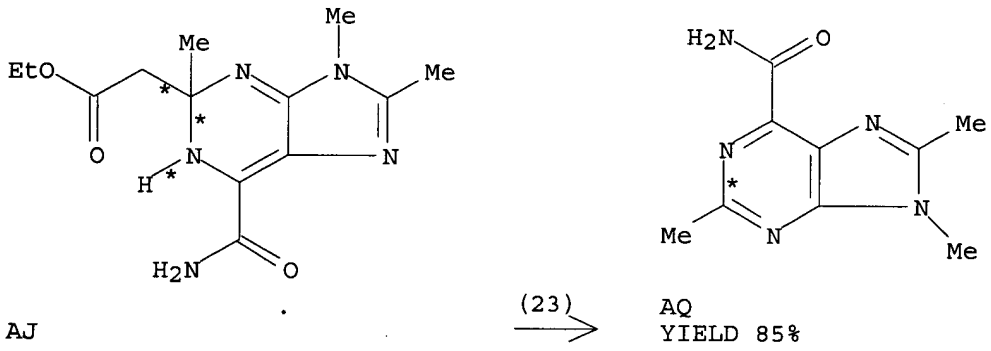
RX(22) OF 78 ...AH ===> AQ



AH → (22) → AQ
YIELD 87%

RX(22) RCT AH 80052-89-7
PRO AQ 80052-82-0
SOL 67-66-3 CHCl3

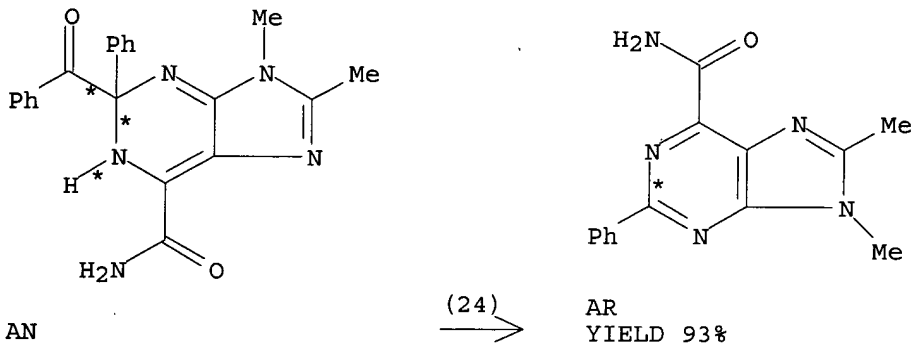
RX(23) OF 78 ...AJ ===> AQ



AJ → (23) → AQ
YIELD 85%

RX(23) RCT AJ 80052-90-0
PRO AQ 80052-82-0
SOL 64-17-5 EtOH

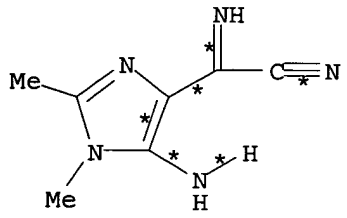
RX(24) OF 78 ...AN ===> AR



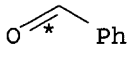
AN → (24) → AR
YIELD 93%

RX(24) RCT AN 80052-92-2
PRO AR 80052-83-1
SOL 67-66-3 CHCl3

RX(25) OF 78 ...Q + AB ===> AS...

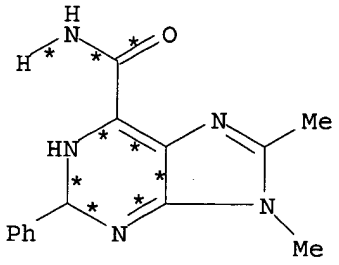


Q



AB

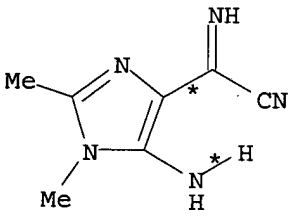
(25)



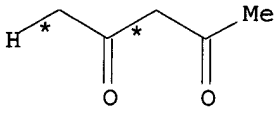
AS
YIELD 97%

RX(25) RCT Q 80052-80-8, AB 100-52-7
PRO AS 80052-93-3
SOL 100-52-7 PhCHO

RX(26) OF 78 ...Q + AT ===> AQ

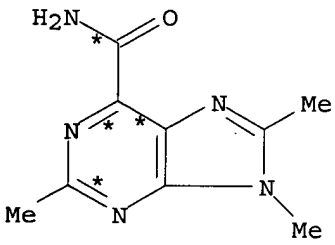


Q



AT

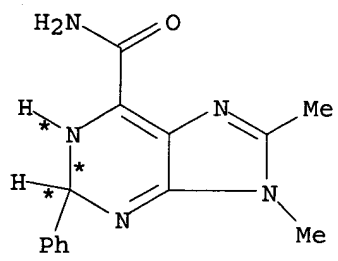
(26)



AQ
YIELD 65%

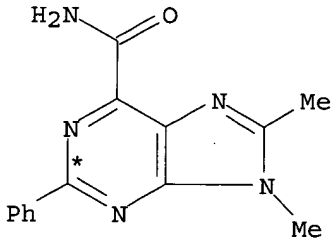
RX(26) RCT Q 80052-80-8, AT 123-54-6
PRO AQ 80052-82-0
SOL 64-17-5 EtOH

RX(27) OF 78 ...AS ===> AR



AS

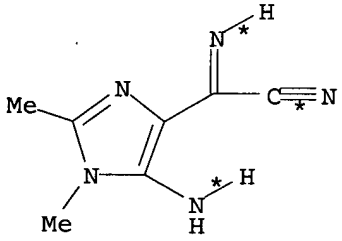
(27)



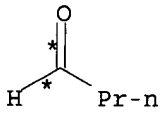
AR
YIELD 59%

RX(27) RCT AS 80052-93-3
PRO AR 80052-83-1
SOL 67-66-3 CHCl3

RX(28) OF 78 ...Q + AU ===> AV

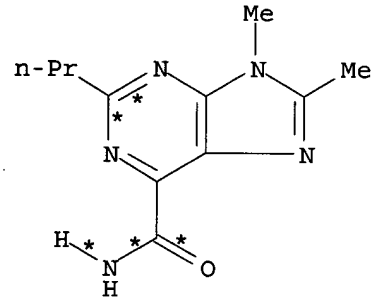


Q



AU

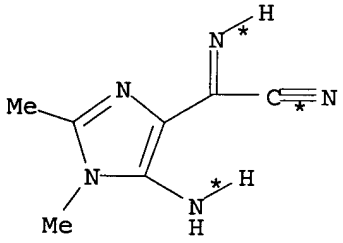
(28)



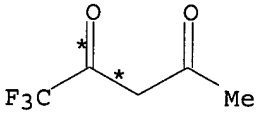
AV
YIELD 93%

RX(28) RCT Q 80052-80-8, AU 123-72-8
PRO AV 80052-85-3

RX(29) OF 78 ...Q + AW ===> AX

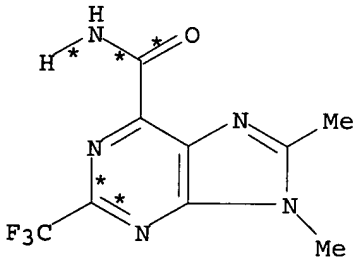


Q



AW

(29) →



AX
YIELD 77%

RX(29) RCT Q 80052-80-8, AW 367-57-7
PRO AX 80052-86-4
SOL 64-17-5 EtOH